

## REPORT DOCUMENTATION PAGE

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14. ABSTRACT  During this funding period, we have completed the PFI-PESICO measurements of the state-selected proton transfer reaction $H_2^+(v^+=0-15, N^+=1) + He(Ne) \rightarrow HeH^+(NeH^+) + H$ . The results of this experiment, together with the cross sections obtained by quasi-classical trajectory (QCT) calculations on this reaction system has been published in the <i>Journal of Chemical Physics</i> (JCP). In a separate theoretical study, which has also been published in JCP, we have performed time-dependent wave-packet calculations on the proton transfer collision of $H_2^+(v^+=0-6, N^+=1) + He$ for comparison with the PFI-PESICO measurements. This theoretical treatment includes the Coriolis coupling (CC) and thus represents the most rigorous theoretical calculation applied to an ion-molecule reaction system. The comparison of the theoretical and experimental cross sections indicates that the inclusion of CC in quantum scattering calculations is important for accurate cross section predictions of ion-molecule reactions. We have also obtained absolute cross sections for the collision-induced dissociation reactions of $HD^+(v^+=0-5) [D_2^+(v^+=0-5)] + He (Ne, Ar, Kr)$ . The manuscripts for these experiments are being prepared for publication. To supplement the PFI-PESICO experiments at the ALS, we have made significant progress in the implementation of the VUV-laser-PFI-PI technique with the TQDO apparatus for state-selected ion-molecule reaction studies.				
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**AFOSR FINAL REPORT (1/2/2003-31/12/2005)**

**I. Grant Title:**

The Chemical Dynamics of Highly vibrationally Excited Diatomic Ions of Aerospace Relevance

**II. Principal Investigators and Addresses**

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**20060405008**

#### IV. Objective:

Numerous Air Force technical environments involve highly nonequilibrium chemistry with hyperthermal collision energies exceeding 10 eV. Since the energies are sufficient to produce electronic excitations and reactive collisions, detailed understanding of the dynamics in this regime is necessary to model the behavior of aerospace systems, such as signatures of spacecraft engine plumes in low-Earth orbit, hypersonic air and reentry plasmas, and the plasmas of electric propulsion thrusters. Quantum reactive scattering efforts at the hyperthermal energies of interest are just beginning to become tractable. Thus, there is a need to validate this work with detailed, state-selected experiments. The main goal of this project is to determine accurate state-selected absolute integral cross-sections for reactions between a series of diatomic ions [ $H_2^+(X^2\Sigma_g^+; v^+, N^+)/HD^+(X^2\Sigma^+; v^+, N^+)/D_2^+(X^2\Sigma_g^+; v^+, N^+)$ ,  $O_2^+(X^2\Pi_{3/2,1/2}, a^4\Pi_u; v^+)$ ,  $NO^+(X^1\Sigma, a^3\Sigma^+; v^+)$ ,  $N_2^+(X^2\Sigma_g^+, v^+)$ , and  $CO^+(X^2\Sigma^+, v^+)$ ] and the rare gas atoms. Particular emphasis is placed on the reaction dynamics involving reactant ions prepared in highly vibrationally excited states, which have not been measured previously. To achieve this goal, we have constructed a unique octopole-quadrupole photoionization apparatus at the advanced Light Source (ALS) and have established the pulsed field ionization-photoelectron-secondary ion coincidence (PFI-PESICO) scheme for absolute total cross section measurements of state-selected ion-molecule processes. The high sensitivity of the PFI-PESICO scheme enables the measurement of absolute cross sections for ion-molecule reactions involving highly vibrationally excited  $H_2^+(X^2\Sigma_g^+; v^+, N^+)/HD^+(X^2\Sigma^+; v^+, N^+)/D_2^+(X^2\Sigma_g^+; v^+, N^+)$  with  $v^+$  close to the dissociation limit of these diatomic ions. However, the PFI-PESICO measurements are highly time-consuming. To supplement the experimental effort at the ALS, we are in the process of developing vacuum ultraviolet (VUV) laser based experiments for state-selected ion-molecule reaction studies at UC Davis by employing the VUV pulsed field ionization-photoion (PFI-PI) method for the preparation of state-selected reactant ions. In order to supply detailed cross section data to model  $Xe^+$  propelled electrostatic thrusters, we also plan to measure absolute spin-orbit-state-selected and resolved total cross sections for the symmetric  $Xe^+(^2P_{3/2,1/2}) + Xe$  charge transfer reaction using the triple-quadrupole-double-octopole (TQDO) photoionization apparatus in our laboratory at UC Davis.

#### V. Status of effort

During this funding period, we have completed the PFI-PESICO measurements of the state-selected proton transfer reaction  $H_2^+(v^+=0-15, N^+=1) + He(Ne) \rightarrow HeH^+(NeH^+) + H$ . The results of this experiment, together with the cross sections obtained by quasi-classical trajectory (QCT) calculations on this reaction system has been published in the *Journal of Chemical Physics* (JCP). In a separate theoretical study, which has also been published in JCP, we have performed time-dependent wave-packet calculations on the proton transfer collision of  $H_2^+(v^+=0-6, N^+=1) + He$  for comparison with the PFI-PESICO measurements. This theoretical treatment includes the Coriolis coupling (CC) and thus represents the most rigorous theoretical calculation applied to an ion-molecule reaction system. The comparison of the theoretical and experimental cross sections indicates that the inclusion of CC in quantum scattering calculations is important for accurate cross section predictions of ion-molecule reactions. We have also obtained absolute cross sections for the collision-induced dissociation reactions of  $HD^+(v^+=0-5) [D_2^+(v^+=0-5)] + He(Ne, Ar, Kr)$ . The manuscripts for these experiments are being prepared for publications. To supplement the PFI-PESICO experiments at the ALS, we have made significant progress in the implementation of the VUV-laser-PFI-PI technique with the TQDO apparatus for state-selected ion-molecule reaction studies.

#### VI. Accomplishments/New Findings:

##### A. Selected scientific findings

The endothermic proton transfer reaction,  $H_2^+(v^+, N^+=1) + Ne \rightarrow NeH^+ + H (\Delta E = 0.54 \text{ eV})$ , has been investigated over a broad range of reactant vibrational energies using the PFI-PESICO scheme. For the lowest vibrational levels,  $v^+ = 0$  and 1, a detailed translational energy dependence is also obtained. Sharp threshold onsets are observed, suggesting the importance of long-lived intermediates or resonances. At a translational energy,  $E_{c.m.} = 0.7 \text{ eV}$ , absolute state-selected reaction cross sections are measured for all reactant vibrational levels  $v^+ = 0 - 17$ . For levels  $v^+ = 0 - 6$ , the cross sections grows rapidly with vibrational quantum, above which the cross section saturates at a value of  $\sim 13 \pm 4 \text{ \AA}^2$ . At levels  $v^+ > 13$ , the cross section declines, probably due to competition with the dissociation channel. At a translational energy,  $E_{c.m.} = 1.7 \text{ eV}$ , absolute state-selected reaction cross sections are measured for reactant vibrational levels spanning the range between  $v^+ = 0$  and 14. Cross section growth is observed from  $v^+ = 0$  to 7, above which the cross sections no longer exhibit a steady trend. At  $E_{c.m.} = 4.5 \text{ eV}$ , cross sections are reported for vibrational levels covering the range between  $v^+ = 0$  and 12. The cross sections are substantially lower at this high translational energy, however, they still exhibit a substantial vibrational enhancement below  $v^+ = 8$ . The present measurements are compared with quasiclassical trajectory

(QCT) calculations. The comparison can be categorized by three distinct total energy ( $E_{\text{tot}} = E_{\text{c.m.}} + E_{\text{vib}}$ ) regimes. For  $E_{\text{tot}} < 1$  eV, the experimental cross sections exceed the QCT results, consistent with important quantum effects at low energies. For  $1 < E_{\text{tot}} < 3$  eV, excellent agreement is observed between the PFI-PESICO cross sections and the QCT calculations. At total energies exceeding 3 eV, the experimental results are generally higher, probably because QCT over predicts competition from the dissociation channel.

The endothermic reaction,  $\text{H}_2^+(\text{v}^+, \text{N}^+=1) + \text{He} \rightarrow \text{HeH}^+ + \text{H}$  is text book system showing the interplay of kinetic and vibrational energy effects on chemical reactivity. We have obtained absolute total cross sections of  $\text{HeH}^+$  for  $\text{v}^+=0-15$  at center-of-mass kinetic energies ( $E_{\text{c.m.}}$ 's) of 0.6 and 3.1 eV. The kinetic energy dependencies of the  $\text{HeH}^+$  cross sections for  $\text{H}_2^+(\text{v}^+=0-3)$  have also been measured. We have performed QCT calculations on the accurate *ab initio* potential energy surface (PES) of Palmieri *et al.* for comparison with experimental cross sections. The QCT proton transfer cross sections for  $\text{H}_2^+ + \text{He}$  are found to be significantly lower than the experimental results near the threshold. At total energies above 2 eV, where quantum effects are less pronounced, the QCT cross sections are in excellent agreement with the experimental cross sections.

In a separate quantum scattering dynamics study, we have carried out the time-dependent wave-packet calculation of the reaction  $\text{H}_2^+(\text{v}^+=2-6, \text{N}^+=1) + \text{He} \rightarrow \text{HeH}^+ + \text{H}$ . This study takes into account the Coriolis coupling (CC) and uses the PES of Palmieri *et al.* The CC total cross sections for the  $\text{v}^+=0-2, 4$ , and 6 states show  $E_{\text{c.m.}}$  dependence behaviors different from those of the previous CS calculation. Furthermore, the  $E_{\text{c.m.}}$  dependencies of the  $\text{HeH}^+$  cross sections based on the CC calculation only exhibit minor oscillations, indicating that the chance is slim for reactive resonances in total cross sections to survive through the partial wave averaging. The magnitude and profile of the CC total cross sections for  $\text{v}^+=0-2$  in the collision energy range of 0.0-2.5 eV are found to be consistent with experimental cross sections. In conclusion, this is the first study to show that the inclusion of Coriolis coupling is important in quantum dynamics scattering calculations of ion-molecule collisions. This theoretical study leads the way for accurate cross section predictions of ion-molecule reactions in the future.

As an ongoing experiment, we have also obtained absolute total cross sections for the CID reactions (1), (2a), and 2(b) in the  $E_{\text{lab}}$  range of 0-10 eV by setting the VUV energies at appropriate autoionization resonances of HD and  $\text{D}_2$  for the preparation of  $\text{HD}^+(\text{X}^2\Sigma^+, \text{v}^+=0-5)$  and  $\text{D}_2^+(\text{X}^2\Sigma_g^+, \text{v}^+=0-5)$ , respectively.



These CID cross sections are consistent with those of  $\text{H}_2^+(\text{v}^+) + \text{Ar}$  obtained previously in our laboratory, indicating that the CID cross section increases significantly as  $\text{v}^+$  is increased. The CID cross sections also reveal a size effect of the neutral reactant, showing a marked increase in  $\text{D}^+/\text{H}^+$  cross sections from He to Ne, to Ar, and to Kr. Pronounced isotopic effect is also observed for the CID cross sections of reactions (2a) and (2b). We have completed QCT calculations on the CID reactions of (1), (2a), and (2b). The time-dependent wave-packet calculation on these reactions is underway.

The detailed comparison of our experimental and theoretical shows that the time-dependent wave-packet calculation including Coriolis coupling is capable of providing accurate reaction cross sections for ion-molecule reactions involving the  $\text{H}_2^+(\text{X}^2\Sigma_g^+; \text{v}^+, \text{N}^+)/\text{HD}^+(\text{X}^2\Sigma^+; \text{v}^+, \text{N}^+)/\text{D}_2^+(\text{X}^2\Sigma_g^+; \text{v}^+, \text{N}^+)$ . Thus, these experimental measurements together with the CC quantum scattering scheme are expected to play an important role for the simulation of complex chemical processes in  $\text{H}_2/\text{D}_2$  discharge plasma.

## B. Experimental accomplishments

Using the TQDO in our laboratory, we have made significant progress in the establishment of VUV laser based state-selected ion-molecule reaction studies by employing the VUV laser PFI-PI approach to prepare state-selected reactant ions. This involves the implementation of the VUV laser PFI techniques with the TQDO apparatus. The greatest advantage of the VUV synchrotron source is the ease of tunability. However, the optical resolution of VUV lasers is more than 10 fold higher than that of the VUV synchrotron sources. Thus, the VUV laser PFI-PI technique offers a higher selectivity for internal states of reactant ions.

For PFI-PI detection using pulsed VUV lasers, PFI-PIs formed from PFI of high- $n$  Rydberg species must be separated from prompt background ions using a dc-separation field and an appropriate time delay between the application of the VUV laser pulse and the pulsed electric field for PFI and ion extraction. The time delay requirement demands lifetime lengthening of high- $n$  Rydberg states, which can be achieved by  $l$ - and  $m$ -mixings induced by Stark electric fields. The practical feature is to apply a small voltage pulse slightly ahead of the VUV laser pulse, such that the ringing of the scrambling voltage pulse due to impedance mismatch extended into time duration of the VUV laser pulse serves to promote the low  $l$ -states originally formed in VUV laser excitation to long-lived high  $l$ -states. Using NO as an example,

we have demonstrated that the intensity of rovibrationally selected  $\text{NO}^+$  ions observed employing the ringing scrambling field PFI-PI scheme can be enhanced by a factor of 5-10.

In order to use the PFI-PIs formed for state-selected ion-molecule reaction studies, it is necessary to reject the prompt ions. We have designed a pulsed voltage scheme for the separation of PFI-PIs and prompt ions. Employing the VUV laser PFI-PI scheme, we have successfully measured the absolute total cross sections for the charge transfer reactions of  $\text{NO}^+(\text{X}^1\Sigma, v^+=0-2) + \text{CH}_3\text{I}$  ( $\text{C}_6\text{H}_6$ ). This manuscript for this demonstration experiment is being prepared for publication.

## VII. Personnel Supported:

1. Professor Cheuk-Yiu Ng:	Principal investigator
2. Dr. Chao Chang	Postdoctoral associate
3. Dr. Hafeng Xu:	Postdoctoral associate
4. Dr. Tao Zhang:	Graduate student (Ph.D. completed Dec/2003)
5. Mr. Xiaonan Tang:	Graduate student (5 <sup>th</sup> year student, Ph.D. to be completed Sept/2006)
6. Mr. Yu Hou	Graduate student (4 <sup>th</sup> year student)
7. Mr. Cassidy Houchins:	Graduate student (3 <sup>rd</sup> year student)

## VIII. Publications (2003-2006):

1. Wenwu Chen, Jianbo Liu, and C. Y. Ng, "Vacuum Ultraviolet Pulsed Field Ionization-Photoelectron Study for  $\text{N}_2\text{O}^+$  in the Energy Range of 16.3 - 21.0 eV", *J. Phys. Chem. A* **107**, 8086-8091 (2003).
2. X.-M. Qian, T. Zhang, P. Wang, and C. Y. Ng, Y. Chiu, D. J. Levandier, J. S. Miller, and R. A. Dressler, "A state-selected study of the  $\text{H}_2^+(\text{X}, v^+=0-17) + \text{Ne}$  proton transfer reaction using the pulsed field ionization-photoelectron-secondary ion coincidence scheme", *J. Chem. Phys.* **119**, 10175-10184 (2003).
3. M. Hochlaf, K.-M. Weitzel, and C. Y. Ng, "Vacuum ultraviolet pulsed field ionization-photoelectron studies of  $\text{H}_2\text{S}$  in the range of 10-16 eV", *J. Chem. Phys.* **120**, 6944 (2004).
4. X.-M. Qian, K.-C. Lau, G.-Z. He, and C. Y. Ng, "Accurate Thermochemistry of the  $\text{ND}_2/\text{ND}_2^+$  and  $\text{ND}_3/\text{ND}_3^+$  Systems", *J. Chem. Phys.* **120**, 8476 (2004).
5. H. K. Woo, P. Wang, K.-C. Lau, X. Xing, and C. Y. Ng, "Single-photon vacuum ultraviolet laser pulsed field ionization-photoelectron studies of *trans*- and *cis*-bromopropenes", *J. Chem. Phys.* **120**, 9561 (2004).
6. X. M. Qian, K. C. Lau, and C.Y. Ng, "A High-Resolution Pulsed Field Ionization-Photoelectron-Photoion Coincidence Study of Vinyl Bromide", *J. Chem. Phys.* **120**, 11031-11041 (2004).
7. H. K. Woo, K.-C. Lau, and C. Y. Ng, "Vibrational spectroscopy of trichloroethene cation by vacuum ultraviolet pulsed field ionization-photoelectron method", *Chinese J. Chem. Phys.* (invited article), **17**, 292 (2004). Selected as the most outstanding article of 2004 by the editorial board of the journal.
8. H. K. Woo, P. Wang, K.-C. Lau, X. Xing, and C. Y. Ng, "VUV pulsed field ionization-photoelectron and VUV-IR-photo-induced Rydberg study of *trans*- $\text{ClCH}=\text{CHCl}$ ", *J. Phys. Chem. A*, **108**, 9637 (2004).
9. P. Wang, X. Xing, K.-C. Lau, H. K. Woo, and C. Y. Ng, "Rovibrationally-state-selected pulsed field ionization-photoelectron study of methyl iodide using two-color infrared-vacuum ultraviolet lasers", *J. Chem. Phys. (Communication)*, **121**, 7049 (2004).
10. P. Wang, X. Xing, S, J, Baek, and C. Y. Ng, "Rovibrationally selected and resolved pulsed field ionization-photoelectron study of ethylene", *J. Phys. Chem. A (Communication)*, **108**, 10035 (2004).
11. C. Y. Ng, "Two-color photoionization and photoelectron studies by combining infrared and vacuum ultraviolet", *J. Electron Spectroscopy & Related Phenomena* (invited review), **142**, 179-192 (2005).
12. Jie Yang, Yuxiang Mo, K. C. Lau, Y. Song, X. M. Qian, and C. Y. Ng, "A combined vacuum ultraviolet laser and synchrotron pulsed field ionization study of  $\text{BCl}_3$ ", *Phys. Chem. Chem. Phys. (Special issue for the 85th International Bunsen Discussion Meeting on Chemical Processes of Ions-Transport and Reactivity)*, **7**, 1518 (2005).
13. X. N. Tang, H. F. Xu, T. Zhang, Y. Hou, C. Chang, C. Y. Ng, Y. Chiu, R. A. Dressler, D. J. Levandier, "A pulsed field ionization photoelectron secondary ion coincidence study of the  $\text{H}_2^+(\text{X}, v^+=0-15, N^+=1) + \text{He}$  proton transfer reaction", *J. Chem. Phys.* **122**, 164301 (2005).
14. K. C. Lau and C. Y. Ng, "Accurate *ab initio* predictions of ionization energies of hydrocarbon radicals:  $\text{CH}_2$ ,  $\text{CH}_3$ ,  $\text{C}_2\text{H}$ ,  $\text{C}_2\text{H}_3$ ,  $\text{C}_2\text{H}_5$ ,  $\text{C}_3\text{H}_3$  and  $\text{C}_3\text{H}_5$ ", *J. Chem. Phys.* **122**, 224310 (2005).

15. T.-S. Chu, R.-F. Lu, K.-L. Han, X.-N. Tang, H.-F. Xu, and C. Y. Ng, "A time-dependent wave packet quantum scattering study of the reaction  $H_2^+(v=0-2, 4, 6; j=1) + He \rightarrow HeH^+ + H$ ", *J. Chem. Phys.* **122**, 244322 (2005).
16. X. N. Tang, Y. Hou, C. Y. Ng, and B. Ruscic, "Pulsed field ionization photoelectron-photoion coincidence study of the process  $N_2 + hv \rightarrow N^+ + N + e^-$ : Bond Dissociation Energies of  $N_2$  and  $N_2^+$ ", *J. Chem. Phys.* **123**, XXXXX (2005).
17. M.-K. Bahng, X. Xing, Sun Jong Baek, and C. Y. Ng, "A two-color infrared-vacuum ultraviolet laser pulsed field ionization photoelectron study of  $NH_3$ ", *J. Chem. Phys.* **123**, 084311 (2005).
18. M. Hochlaf, T. Baer, X. M. Qian, and C. Y. Ng, "A Photoionization and Pulsed Field Ionization-Photoelectron Study of Cyanogen", *J. Chem. Phys.* **123**, 144302 (2005).
19. Tao Zhang, C. Y. Ng, Chow-Shing Lam, and Wai-Kee Li, "A 193 nm Laser Photofragmentation Time-of-Flight Mass Spectrometric Study of  $CH_2ICl$ ", *J. Chem. Phys.* **123**, 174316 (2005).
20. M.-K. Bahng, X. Xing, Sun Jong Baek, X.-M. Qian, and C. Y. Ng, "A combined VUV synchrotron pulsed field ionization-photoelectron and IR-VUV laser photoion depletion study of ammonia", *J. Phys. Chem. A*, web published Dec. 6, 2005.
21. Jingang Zhou, Kai-Chung Lau, Elsayed Hassanein, Haifeng Xu, Shan-Xi Tian, Brant Jones, and C. Y. Ng, "A photodissociation study of  $CH_2BrCl$  in the A-band using the time-sliced velocity ion imaging method", *J. Chem. Phys.* **124**, 034309 (2006).
22. K.-C. Lau and C. Y. Ng, "Accurate *ab initio* predictions of ionization energies and heats of formation for the 2- $C_3H_7$ ,  $C_6H_5$ , and  $C_7H_7$  radicals", *J. Chem. Phys.* **124**, 044323 (2006).
23. P. Wang, H. K. Woo, K. C. Lau, X. Xing, C. Y. Ng, A. S. Zyubin, and A. M. Mebel, "Infrared vibrational spectroscopy of *cis*-dichloroethene in excited Rydberg states", *J. Chem. Phys.* **124**, 064310 (2006).
24. T. Zhang, X. N. Tang, K.-C. Lau, C. Y. Ng, C. Nicolas, D. S. Peterka, M. Ahmed, M. L. Morton, B. Ruscic, R. Yang, L. X. Wei, C. Q. Huang, B. Yang, J. Wang, L. S. Sheng, Y. W. Zhang, and F. Qi, "Direct identification of propargyl radical in combustion flames by VUV photoionization mass spectrometry", *J. Chem. Phys.* **124**, 074302 (2006).
25. K.-C. Lau and C. Y. Ng, "Accurate *ab initio* predictions of ionization energies and heats of formation for the cyclopropenylidene, propargylene and propadienylidene radicals", *Chinese Journal of Chemical Physics* (invited article), **19**, 29-38 (2006).
26. H. K. Woo, K. C. Lau, P. Wang, X. Xing, and C. Y. Ng, "Vacuum ultraviolet laser pulsed field ionization-photoelectron study of *cis*-dichloroethene", *J. Chem. Phys.*, submitted.
27. Kai-Chung Lau and Cheuk-Yiu Ng, "Benchmarking high-level *ab initio* thermochemical predictions with accurate pulsed-field ionization photoion-photoelectron measurements", *Accounts on Chemical Research* (invited article), submitted.

## IX. Interactions/Transitions:

### A. Invited talks at workshops, conferences, and seminars (2003-present)

1. C. Y. Ng, "Opportunities in the Application of FEL for atomic and Chemical Physics Studies", Plenary session presentation (invited), Workshop on *Argonne Free Electron Laser Facility*, Oct. 30, 31, 2003.
2. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics by High-Resolution Photoionization and Photoelectron Methods" (invited), Department of Chemistry, University of California at San Diego, Dec. 2, 2003.
3. T. Zhang, X. Qian, C. Y. Ng, Y.-H. Chiu, D. J. Levandier, J. S. Miller, and R. A. Dressler, "Reactions of state-selected  $H_2^+(X, v^+=0-17, N^+=1)$  with Ne and Ar: A pulsed field ionization-photoelectron-secondary ion coincidence study" (selected as a hot topic for presentation), *SASP04, the 14th Symposium on Atomic, Cluster and Surface Physics*, La Thuile (Aosta), Italy, Feb. 1-6, 2004, presented by D. J. Levandier.
4. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics by High-Resolution Photoionization and Photoelectron Methods" (invited), Department of Chemistry, The Chinese University of Hong Kong, "Symposium in honor of the retirement of Prof. C. W. Mak", Feb. 20, 2004.
5. C. Y. Ng, "Vacuum Ultraviolet Spectroscopy and Chemistry by High-Resolution Photoionization and Photoelectron Methods" (invited), Institute for Atomic and Molecular Sciences, Taipei, Taiwan, March 18, 2004.
6. C. Y. Ng, "High-Resolution State-Selected Ion-Molecule Reaction Studies Using Pulsed Field Ionization Photoelectron-Secondary Ion Coincidence Method", AFOSR Molecular Dynamics Contractors' Meeting (invited), Newport, RI, May 24-26, 2004.
7. C. Y. Ng, "Vacuum Ultraviolet Spectroscopy and Chemistry by High-Resolution Photoionization and Photoelectron Methods" (invited), Air Force Research Lab., Hanscom, Boston, May 27, 2004.

8. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics by High-Resolution Photoionization and Photoelectron Methods", Plenary Lecture (invited), *International Conference on Physics Education and Frontier Research*, Shanghai, China, June 28-July 1, 2004.
9. C. Y. Ng, "Two-color photoionization and photoelectron studies by combining infrared and vacuum ultraviolet" (invited), *Symposium on Molecular Reaction Dynamics*, Dalian, China, July 20-23, 2004.
10. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics by High-Resolution Photoionization and Photoelectron Methods" (invited), *Workshop on Frontiers in Photoionization and Ion-Molecule Reaction Dynamics*, Technical University of Chemnitz, Germany, July 27, 2004.
11. C. Y. Ng, "State-selected ion-molecule reaction studies using the high-resolution pulsed field ionization-photoelectron-secondary ion coincidence method" (invited Plenary Lecture), *The 85th internationally Bunsen Discussion Meeting on Chemical of processes of ions - transport and reactivity*, University of Marburg, Germany, Sept. 15-17, 2004.
12. Peng Wang, Xi Xing, Kai-Chung Lau, and C. Y. Ng, "Two-color photoionization-photoelectron spectroscopy using tunable vacuum ultraviolet and infrared lasers" (selected as a hot topic for oral presentation), *52nd Annual Western Spectroscopy Association Conference*, Asiloma, CA, Jan 26-29, 2005, presented by Peng Wang.
13. X.-M. Qian, C. Y. Ng, and F. Merkt, "IR-VUV Double Resonance", *Third Swiss Snow Symposium for Young Chemists*, Stechelerg, Switzerland, Feb. 18-20, 2005, presented by X.-M. Qian.
14. C. Y. Ng, "Vacuum Ultraviolet Photoionization and Photoelectron Spectroscopy and Dynamics", *Workshop on Free Electron Laser*, Duke University, Feb. 23-25, 2005.
15. C. Y. Ng, "Unimolecular and Bimolecular Reaction Dynamics of State-Selected Ions by Pulsed Field Ionization Method", *SOLEIL Workshop on "New trends in gas phase VUV/Soft X-ray high resolution spectroscopy at SOLEIL"*, 21-22 March 2005, Universite Paris-Sud, Orsay, France.
16. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics by High-Resolution Photoionization and Photoelectron Methods", Department of Chemistry, University of Southern California, March 28, 2005.
17. C. Y. Ng, "Frontier in Photoionization and Photoelectron Studies: Recent Developments and Future Prospects" (invited Plenary Lecture), International Conference on "Next 100 Years of Physics and Its Impacts on Engineering, lifesciences and technology". The National Nanyang University and National Singapore University, Singapore, Aug. 10-12, 2005.
18. "State-Selected and State-to-State Photoionization-Photoelectron Spectroscopy using Two-Color Infrared and Vacuum Ultraviolet Lasers", Pacific Northwest National Laboratory, Sept. 9, 2005. Presented by Peng Wang.
19. C. Y. Ng, "Two-Color Photoionization-Photoelectron Studies by Combining Infrared and Vacuum Ultraviolet", The 9th National Conference of Chemical Reaction Kinetics", Hangzhou, China, Sept. 24-27, 2005.
20. "High-Resolution Photoelectron and Photoion Spectroscopy of Ammonia using Two-Color Infrared-Vacuum Ultraviolet Lasers", Chemistry Division, Argonne National Laboratory, Sept. 27, 2005. Presented by MiKyung Bahng.
21. C. Y. Ng, "Frontier in Vacuum Ultraviolet Photoion-Photoelectron Studies: Recent Developments and Future Prospects", Dalian Institute of Chemical Physics, China. Oct. 12, 2005.
22. C. Y. Ng, "Frontier in Photoionization and Photoelectron Studies: Recent Developments and Future Prospects", USTC Conference, University of Science and Technology of China, Hefei, China, Nov. 17-18, 2005.
23. C. Y. Ng, "High-resolution photoion and photoelectron studies at the Advanced Light Source", Workshop on Synchrotron Radiation Research from Infrared to Soft x-ray", National Synchrotron Radiation Laboratory, USTC, Nov. 19 and 20, 2005.
24. C. Y. Ng, "Two-color Infrared-Vacuum Laser Ultraviolet photoion-photoelectron studies", Gordon Research Conference on "Photoions, Photoionization and Photodetachment", Santa Ynez Valley Mariot, Buellton, CA, Jan 31-Feb. 3, 2006.
25. "State-Selected Ion Molecule Reactions", Chemical Dynamics Beamline Review, Lawrence Berkeley Laboratory, Berkeley, CA, Feb. 28, 2006. Presented by Rainer A. Dressler.

#### B. Interactions

This project represents a collaborative project between our group at UC Davis and Dr. Rainer Dressler's group at the Hanscom Air Force Research laboratory.

#### C. Transitions

The thermochemical data obtained by our group based on VUV photoion and photoelectron measurements have been used by the "Active Thermochemical Table" project (project leader: Dr. Branko Ruscic) of the Argonne National Laboratory. This project is supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic

Energy Sciences. The absolute state-selected total cross sections for the ion-molecule reactions of O<sup>+</sup>(<sup>4</sup>S, <sup>2</sup>D, <sup>2</sup>P) + H<sub>2</sub>O (N<sub>2</sub>, CO<sub>2</sub>, O<sub>2</sub>) have been used by NASA for modeling the chemistry of planetary atmospheres.

**X. New Discoveries:**

None

**XI. Honors/Awards:**

**Lifetime achievement honors**

2005	Elected Fellow, American Association for the Advancement of Sciences
2003	Distinguished Professor, UC Davis
1998	Alexander von Humboldt Senior Scientist Award
1997	Senior Fellow, Japanese Society for the Promotion of Science
1996	Distinguished Professor of Liberal Arts and Sciences, Iowa State University
1994	Iowa Regents Award for Faculty Excellence
1993	Elected Fellow, American Physical Society
1985	Honorary Professor of Chemistry, Zhengzhou University, China
1982	Camille and Henry Dreyfus Teacher-Scholar
1981	Alfred P. Sloan Foundation Fellow